Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Theoretical Studies on the Transport Mechanism of 5-Fluorouracil through Cyclic Peptide Based Nanotubes

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Electronic Supplementary Information:

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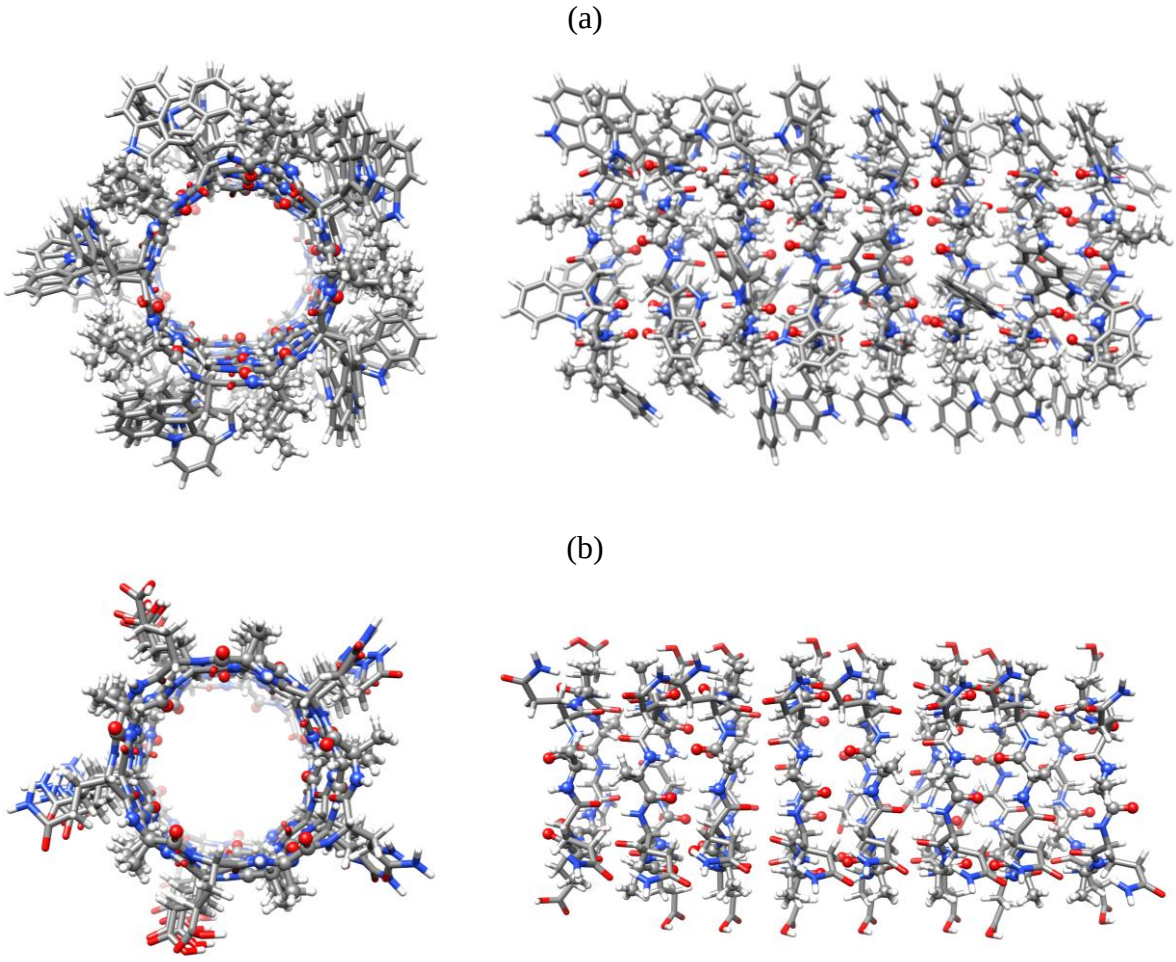


Figure S1: Model structures of {*cyclo*-[(D-Trp-L-Leu)$_5$]}$_8$ (a) and {*cyclo*-[(L-Ala-D-Gln-L-Ala-D-Glu)$_2$-L-Ala-D-Gln]}$_8$ (b) system. The Leu and Ala amino acids are shown with ball and stick representation.

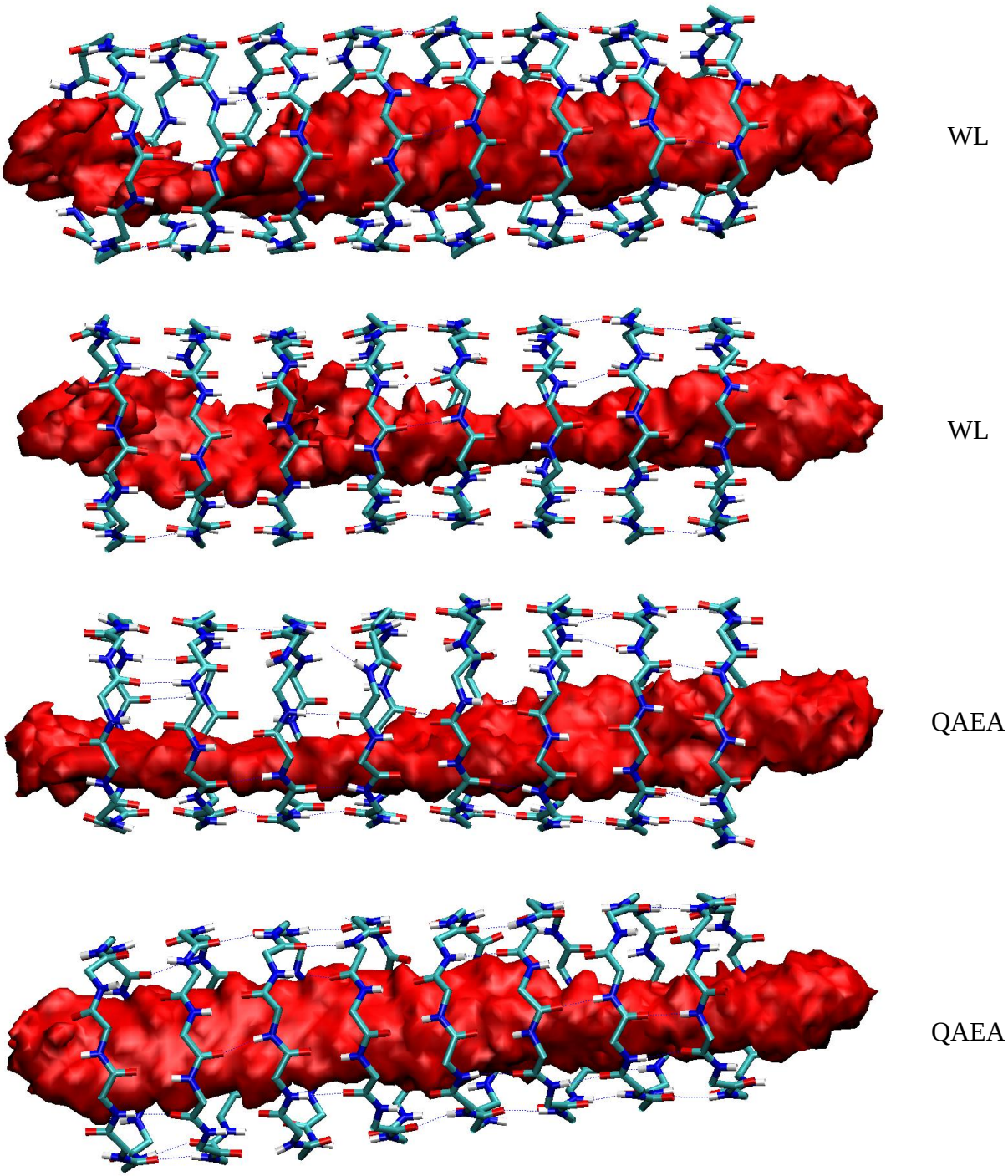
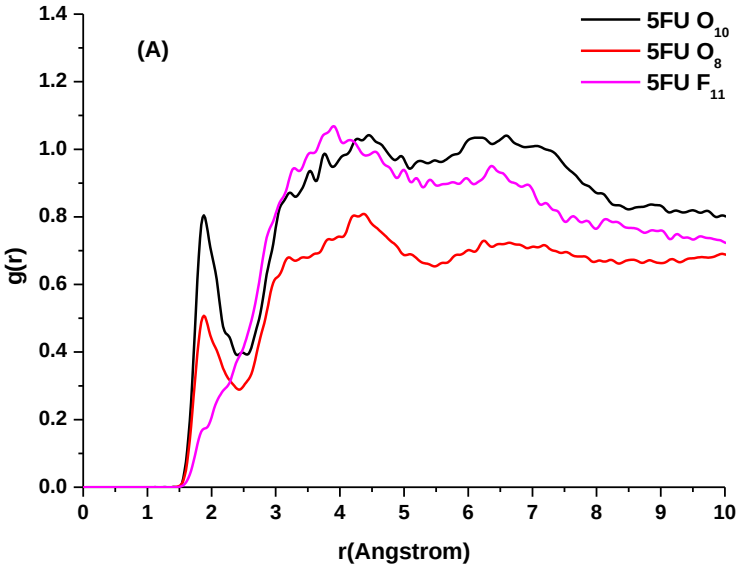
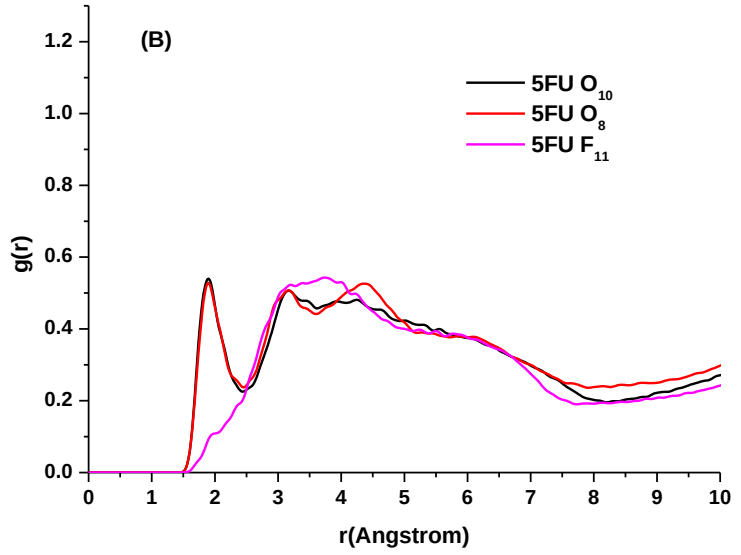


Figure S2: The spatial distribution function of 5FU during its transport through WL and QAEA systems. The amino acid side chains are not shown for clear visibility and the intermolecular H-bonding is represented as dotted lines.


(A)
5FU O10
5FU O8
5FU F11
g(r)
r(Angstrom)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
1
2
3
4
5
6
7
8
9
10


(B)
5FU O10
5FU O8
5FU F11
g(r)
r(Angstrom)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0
1
2
3
4
5
6
7
8
9
10

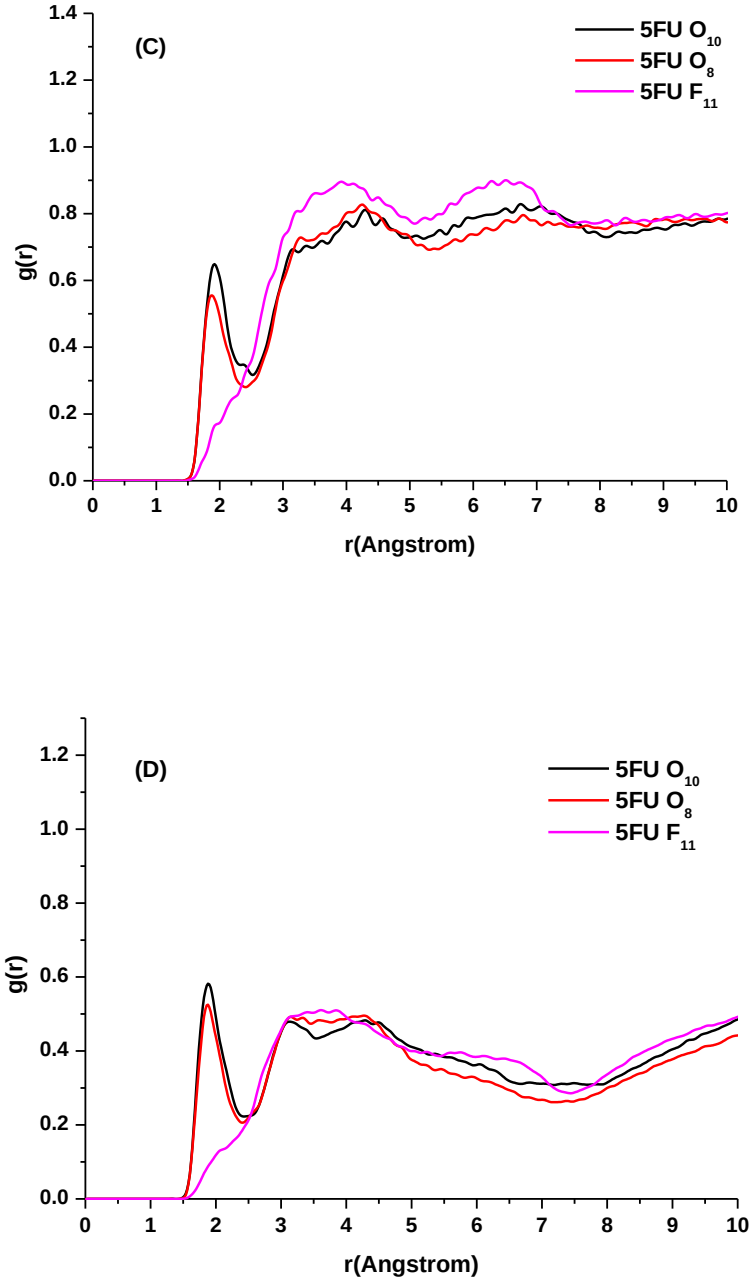


Figure S3: Radial pair distribution functions g(r) between various atoms of 5FU and water H atoms of WL (A, B) and QAEA (C, D) systems. The densities as observed in the bulk water (A, C) and in the diffusion pathway (B, D).

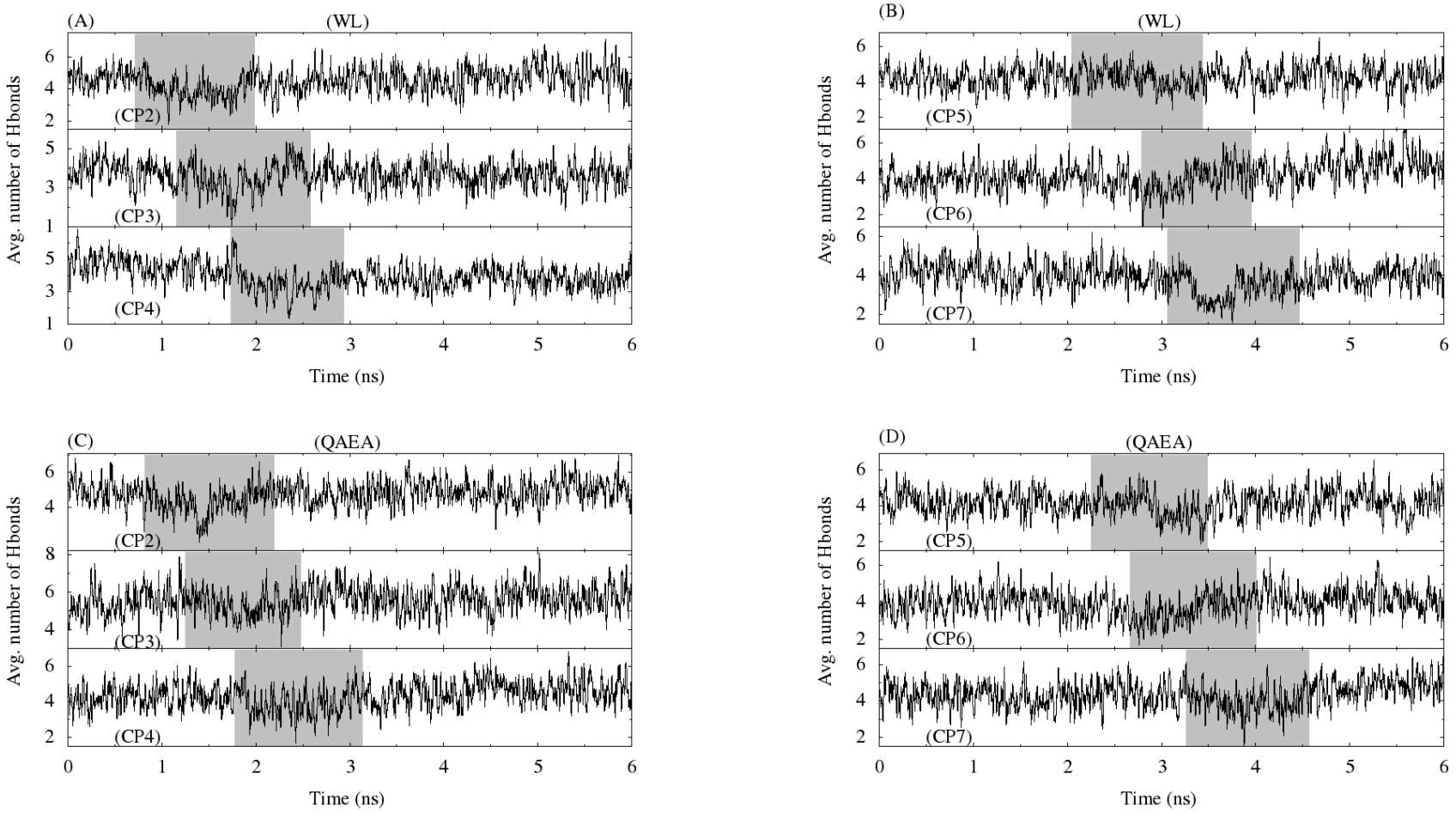


Figure S4: The running average (window size 50) of number of H-bonds between water molecules and backbone carbonyl O atoms of various CPs from WL (A) and QAEA (B) systems as observed from the SMD simulation. The existence of van der Waals contact (with cut off distance of < 3.5 Å) between 5FU and various CP units are represented with grey colour.

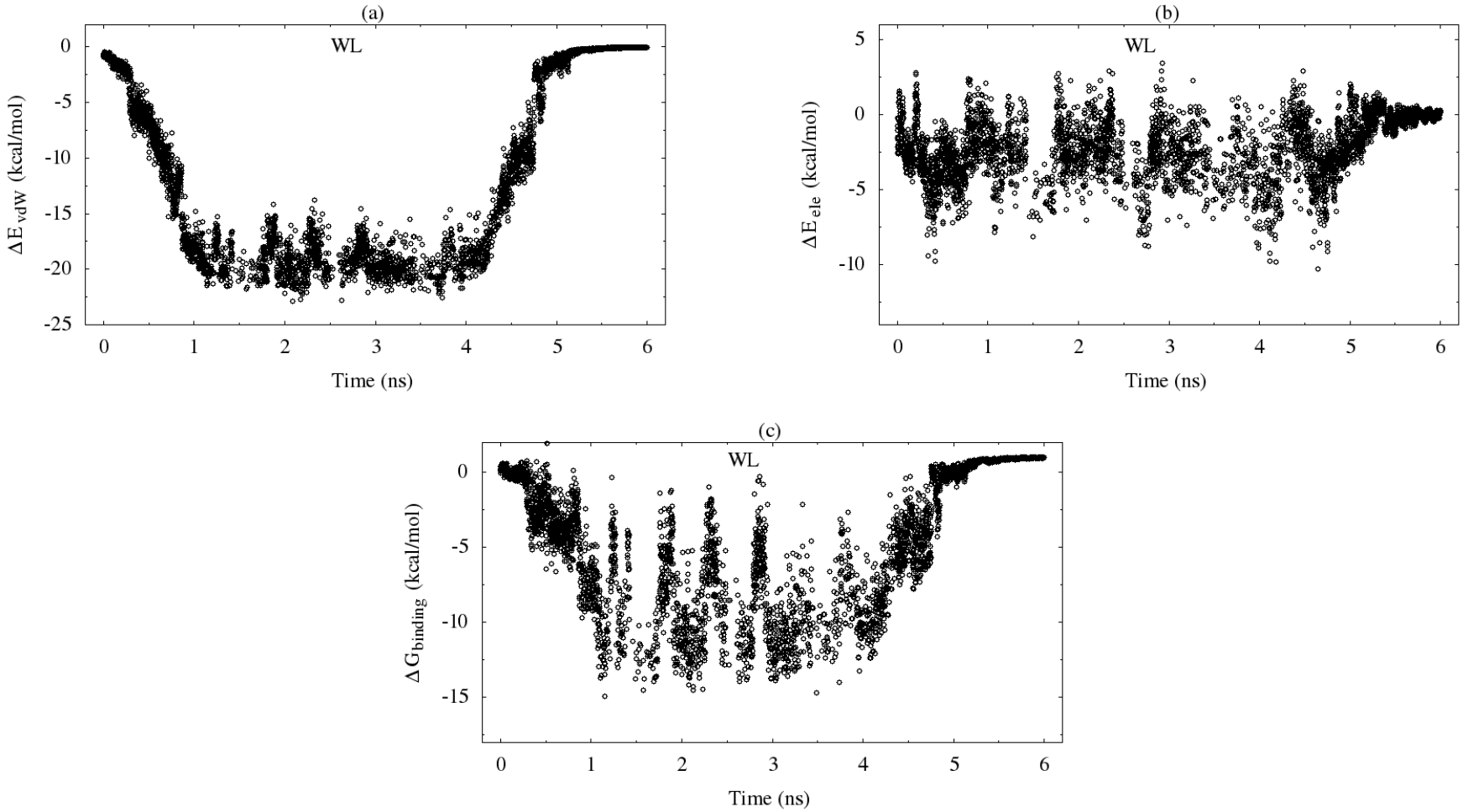


Figure S5: (a) van der Waals and (b) electrostatic energy contributions to the (c) free energy of binding of non H-bonded CPNT-5FU complex structures extracted from the SMD simulation of WL system.

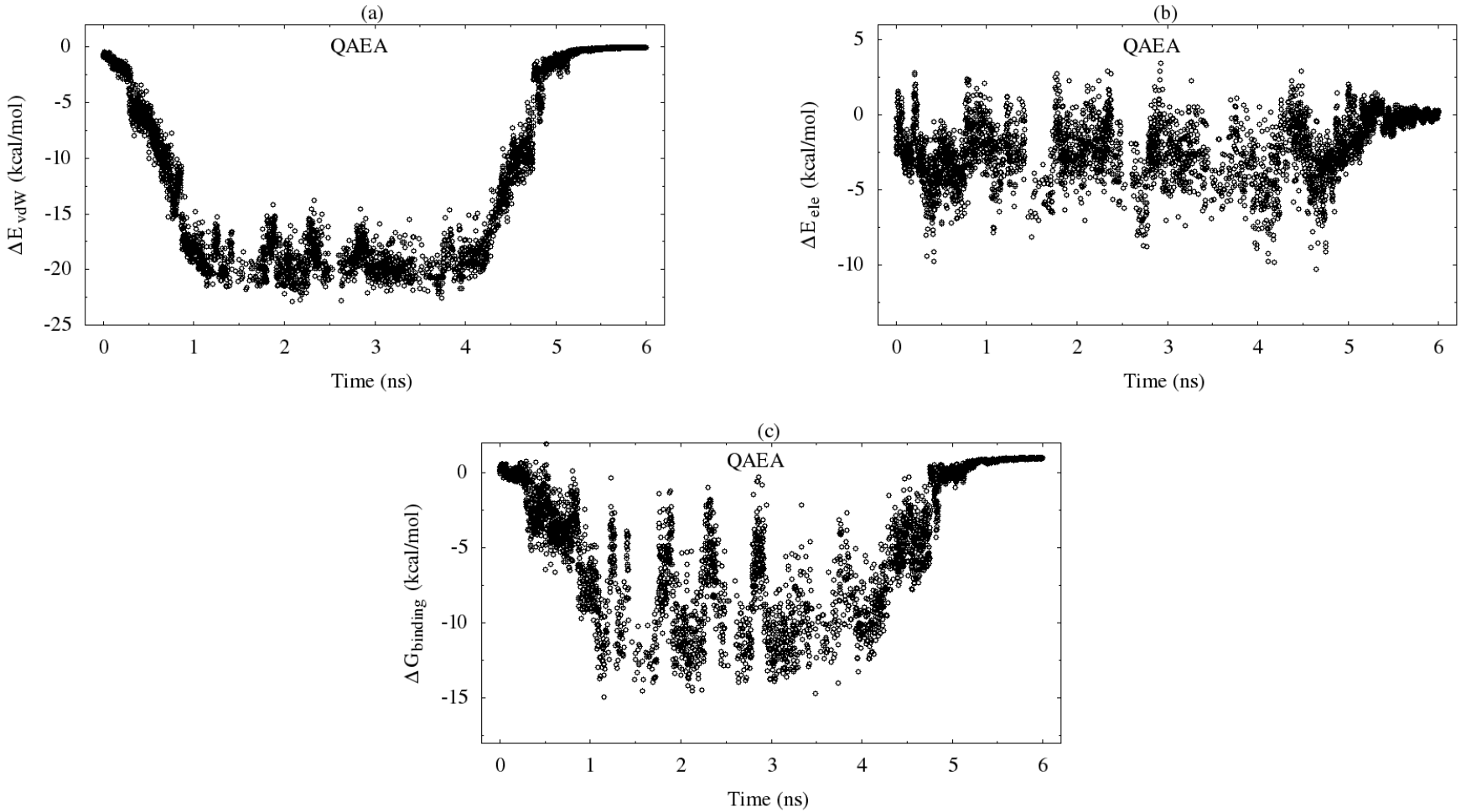


Figure S6: (a) van der Waals and (b) electrostatic energy contributions to the (c) free energy of binding of non H-boned CPNT-5FU complex structures extracted from the SMD simulation of QAEA system.

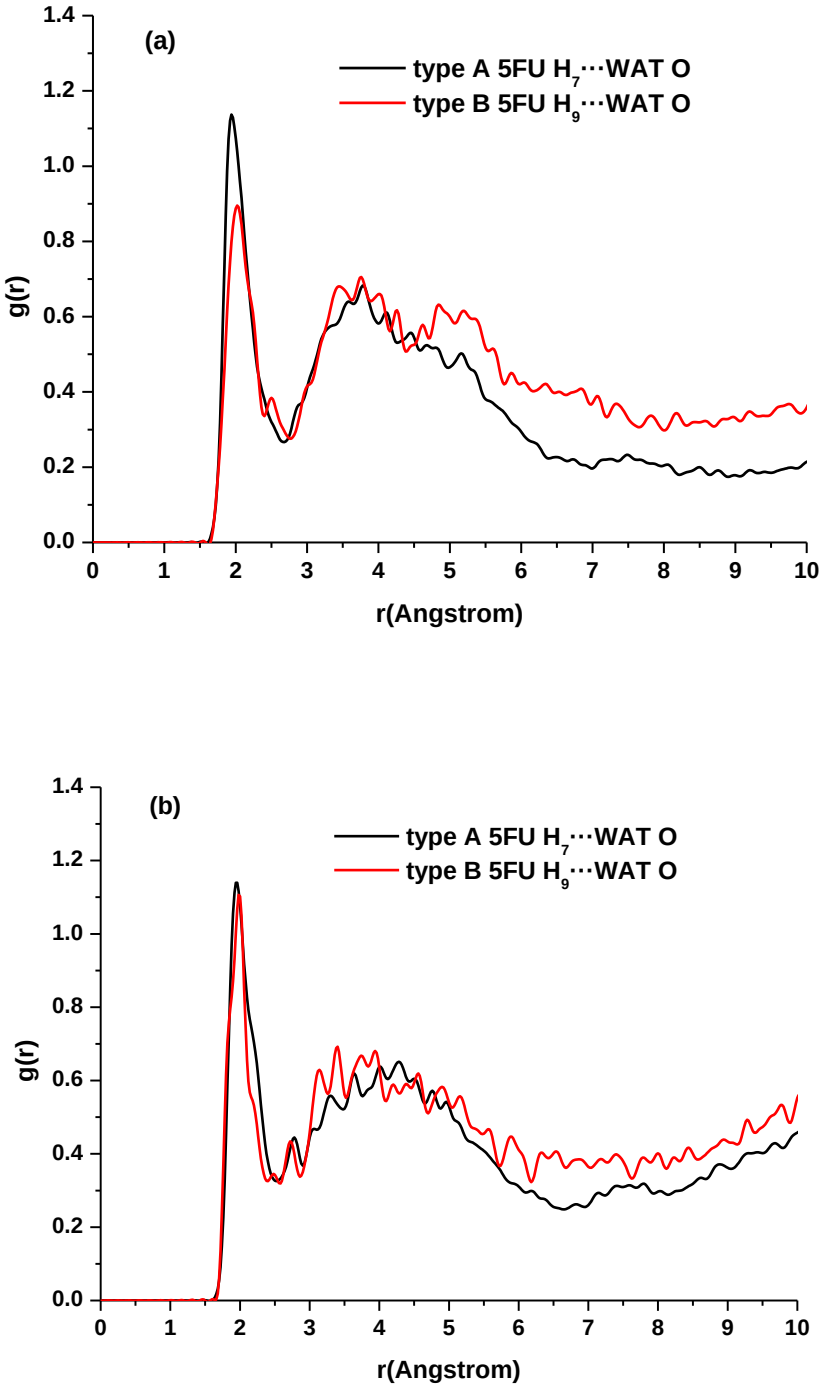


Figure S7: Radial distribution function of water O around 5FU H_7/H_9 atoms in the presence of type A and B H-bonds observed from the WL (a) and QAEA (b) systems.

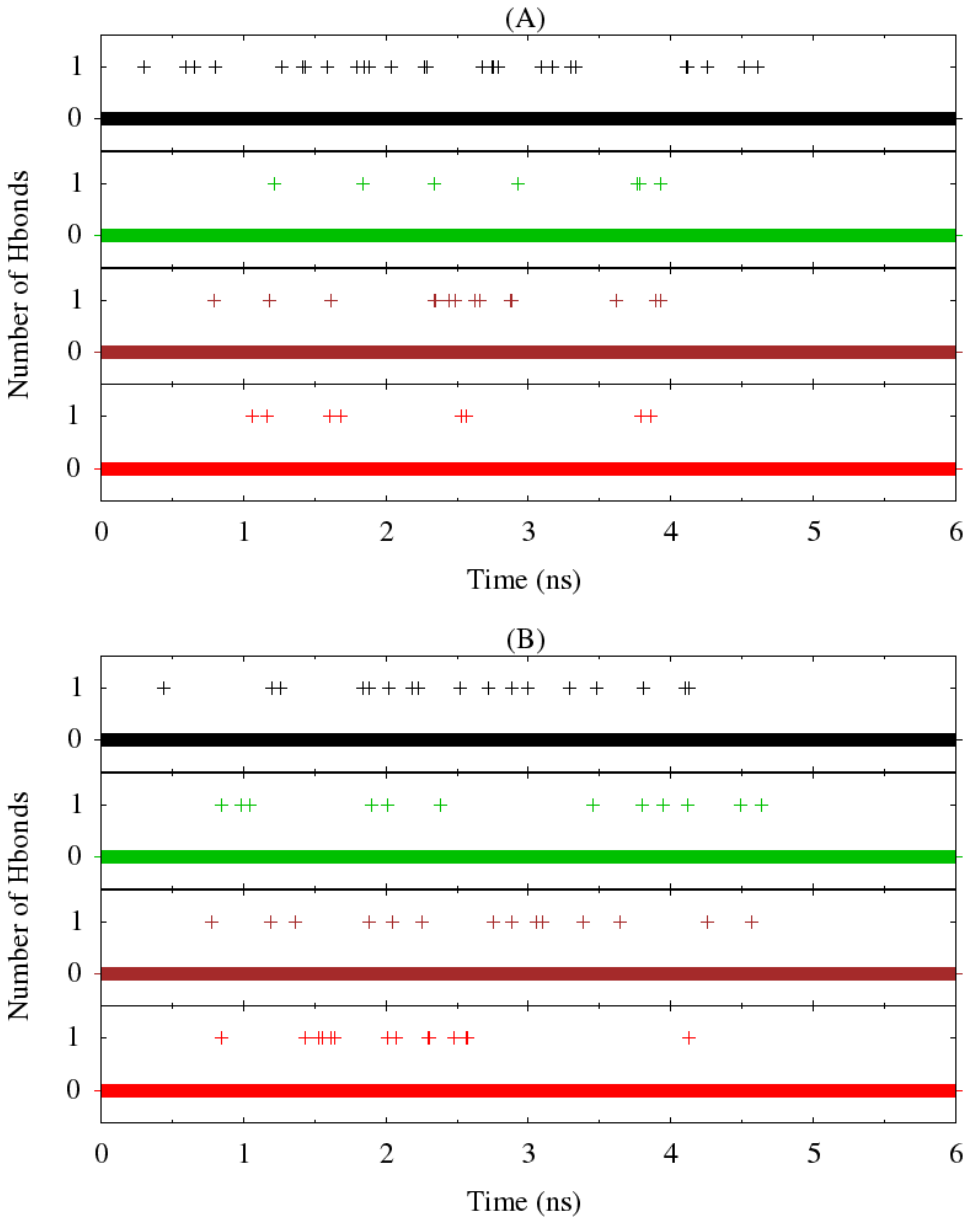


Figure S8: Water mediated H-bonds between CPNT amide N and various atoms of 5FU observed from the WL (A) and QAEA (B) systems. H-bonds: N(CPNT)···H–O(WAT)···N_1H_7(5FU) (black), N(CPNT)···H–O(WAT)···N_3H_9(5FU) (Green), N(CPNT)···H–O–H(WAT)···O_8(5FU) (Brown), N(CPNT)···H–O–H(WAT)···O_{10}(5FU) (Red).

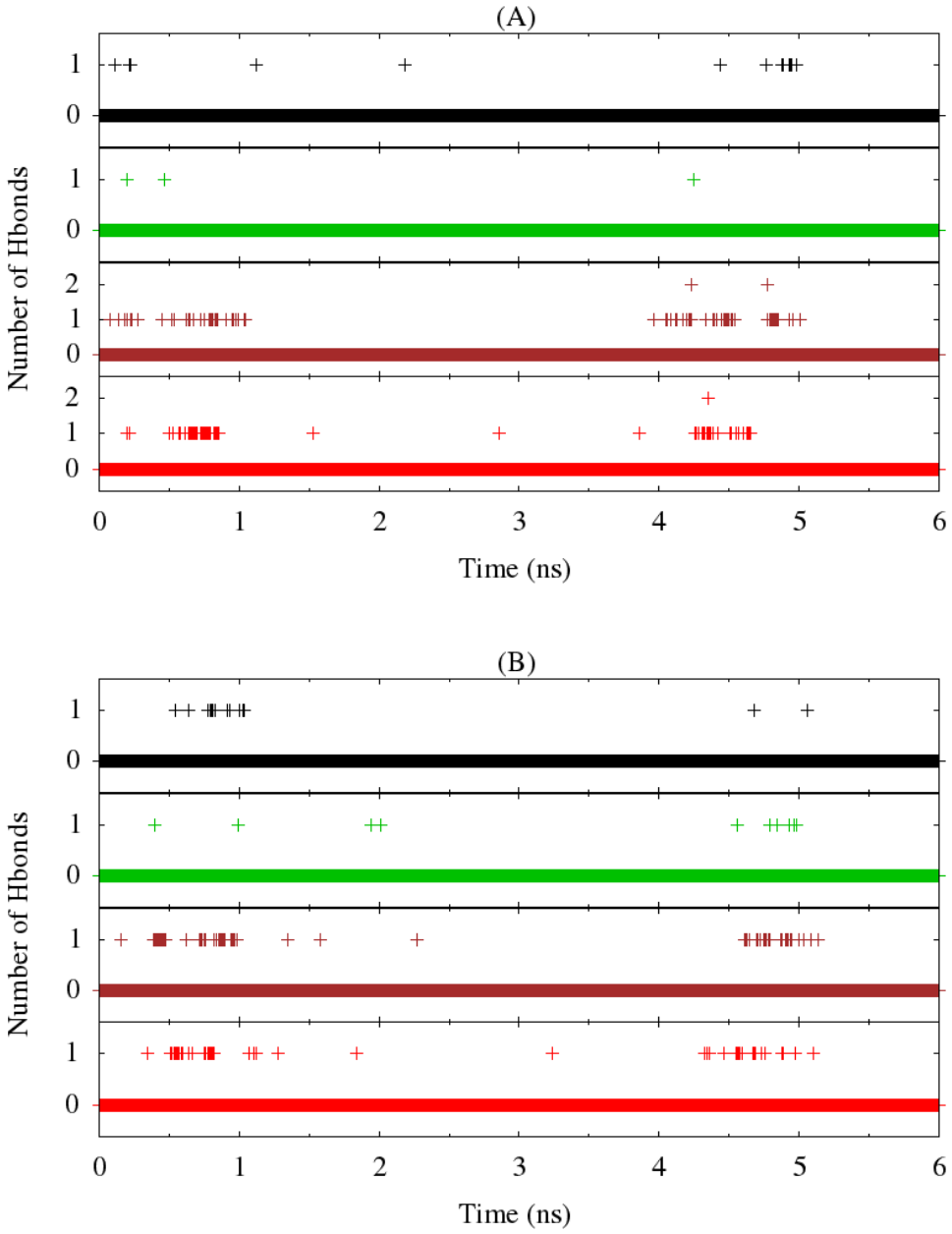


Figure S9: Water mediated H-bonds between CPNT amide NH and various atoms of 5FU observed from the WL (A) and QAEA (B) systems. H-bonds: NH(CPNT)···O(WAT)···N_1H_7(5FU) (black), NH(CPNT)···O(WAT)···N_3H_9(5FU) (Green), NH(CPNT)···O–H(WAT)···O_8(5FU) (Brown), NH(CPNT)···O–H(WAT)···O_{10}(5FU) (Red).